

1,1,2,2-Tetrafluoro-2-(1,1,2,2-tetrafluoroethoxy)ethane-1-sulfonyl fluoride
104729-49-9 | DTXSID40446988

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 334 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.13e-01

Confidence level: 5.47e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chlorothalonil</div> <div>Measured: 1820</div> <div>Predicted: 1300</div>	<div>Image not found</div> <div>Chloranil</div> <div>Measured: 209</div> <div>Predicted: 259</div>	<div>Image not found</div> <div>Sulfone, methyl pentafluorophenyl</div> <div>Measured: 28.8</div> <div>Predicted: 104</div>
<div>Image not found</div> <div>Tetrachlorophthalic acid</div> <div>Measured: 2000</div> <div>Predicted: 1980</div>	<div>Image not found</div> <div>Naled</div> <div>Measured: 182</div> <div>Predicted: 184</div>	